Propanedioic acid, 1,3-dithiolan-2-ylidene-, bis(1-methylethyl) ester

Other names: Di-isopropyl 1,3-dithiolane-2-ylidenemalonate
Fudiolan
Fuji 1
Fujione
IPT
Isoprothiolane
NKK 100
NNF-109
SS 11946
IPT (pesticide)
Bis(1-methylethyl) 1,3-dithiolan-2-ylidenepropanedioate
Diisopropyl 2-(1,3-dithiolan-2-ylidene)propanedioate
Malonic acid, 2-(1,3-dithiolan-2-ylidene), diisopropyl ester
Propanedioic acid, 2-(1,3-dithiolan-2-ylidene)-, 1,3-bis(1-methylethyl) ester

Inchi: InChI=1S/C12H18O4S2/c1-7(2)15-10(13)9(11(14)16-8(3)4)12-17-5-6-18-12/h7-8H,5-6H2

InchiKey: UFHLMYOGRXOCSL-UHFFFAOYSA-N

Formula: C12H18O4S2

SMILES: CC(C)OC(=O)C(C(=O)OC(C)C)=C1SCCS1

Mol. weight [g/mol]: 290.40

CAS: 50512-35-1

Physical Properties

Property code	Value	Unit	Source
gf	-261.67	kJ/mol	Joback Method
hf	-553.59	kJ/mol	Joback Method
hfus	24.56	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.581		Crippen Method
mcvol	212.360	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	2194.00		NIST Webbook
rinpol	2198.00		NIST Webbook
rinpol	2177.00		NIST Webbook
tb	747.79	K	Joback Method
tc	981.23	K	Joback Method
tf	517.76	K	Joback Method

vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.55	J/mol×K	747.79	Joback Method
cpg	588.07	J/mol×K	786.70	Joback Method
cpg	601.53	J/mol×K	825.60	Joback Method
cpg	613.95	J/mol×K	864.51	Joback Method
cpg	625.36	J/mol×K	903.41	Joback Method
cpg	635.81	J/mol×K	942.32	Joback Method
cpg	645.32	J/mol×K	981.23	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50512351&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume